

1.1.17 Shape of s-orbitals, node and nodal surface

The expression for angular wave function for s-orbital is not dependent on either of the θ or ϕ . In other words, the angular part of the wave function is spherically symmetrical. Thus probability of finding the electron is equal in all directions. Keeping in mind that atoms are three-dimensional, the probability surface diagram of s-orbital is spherical Fig. 1.16.

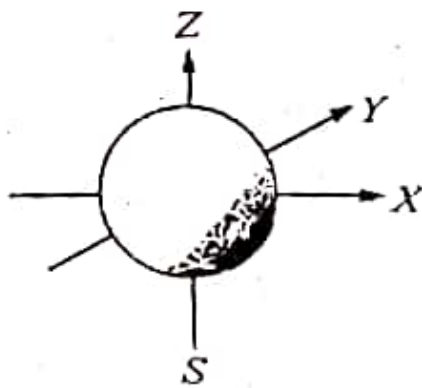


Fig. 1.16.

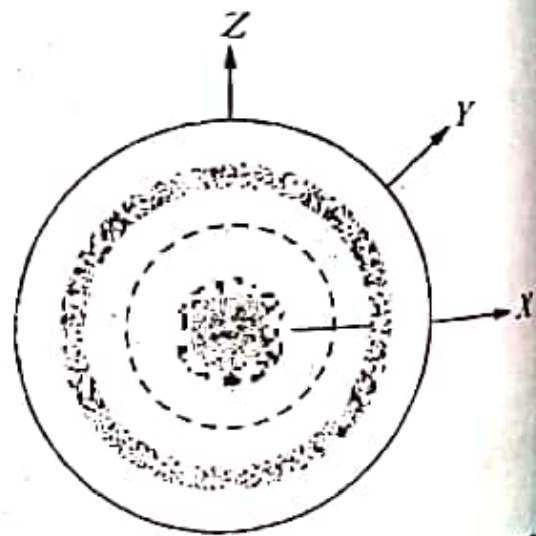


Fig. 1.17. Dot representation of electron density in 2s orbital.

In the radial distribution curve for 2s-orbital there are two regions of high probability separated by a node at $r = r_1$. Fig. 1.17 for 2s shows two regions of higher dot density separated by a spherical nodal surface (shown as dotted circle) at distance r_1 from the nucleus.

Such diagrams showing nodal surfaces will be avoided because by doing so we are extending the mathematical model to too much of simplification. The wave model prevents us firstly to locate the electron as a particle in one region and then explain its motion to the other region through an intervening nodal surface. For such a visualization, the electron as standing wave would be more appropriate because such a wave can exist simultaneously on both sides of nodes.

1.1.18 Shape of p -orbitals

For $l = 1$, m has three values, $\pm 1, 0$ representing the three orientations of p -orbitals, p_x, p_y, p_z .

Angular wave function for $l = 1, m = 0$ is labelled as p_z and the expression $\left[\frac{3}{4}\pi\right]^{1/2} \cos \theta$ gives two tangent dumb-bells symmetrical about Z -axis. In other words, the angular part of the probability distribution is concentrated along Z -axis and the resulting surface of p_z electron has the form of a dumb-bell along the Z -axis. The dumb-bell shaped lobes of high probability are separated by a nodal surface in XY -plane. Other two orbitals p_x and p_y have similarly been found to have dumb-bell shapes along X and Y -axis, respectively as shown in Fig. 1.18. The electron in a p -orbital is found with equal probability in either of the lobes. The three p -orbitals p_x, p_y and p_z together having an electron in each one of these give a spherical distribution of electron density.

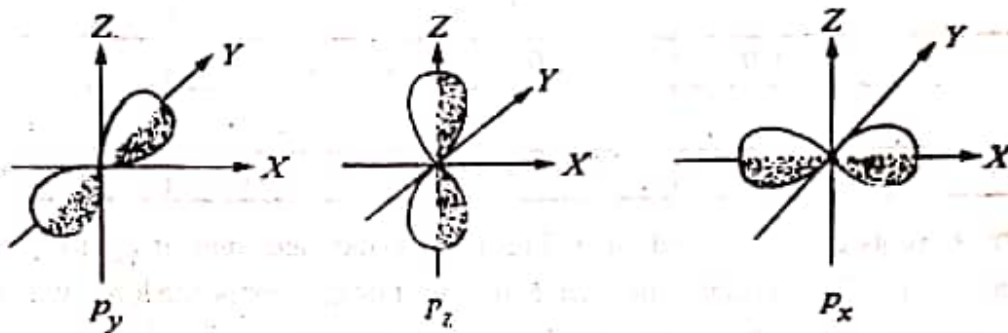


Fig. 1.18. Shape of p -orbitals.

1.1.19 Shape of d -orbitals

For $l = 2$, m has five values $0, \pm 1, \pm 2$ representing the five orientations of d -orbitals designated as $d_{z^2}, d_{x^2-y^2}, d_{xy}, d_{yz}, d_{zx}$, as shown in Fig. 1.19. Their angular dependence is more complicated than that of p -orbital. Probability surface diagrams of three orbitals d_{xy}, d_{yz} and d_{zx} have four lobes of high electron density in xy, yz and zx planes respectively with each lobe bisecting the principal axis into two equal halves.

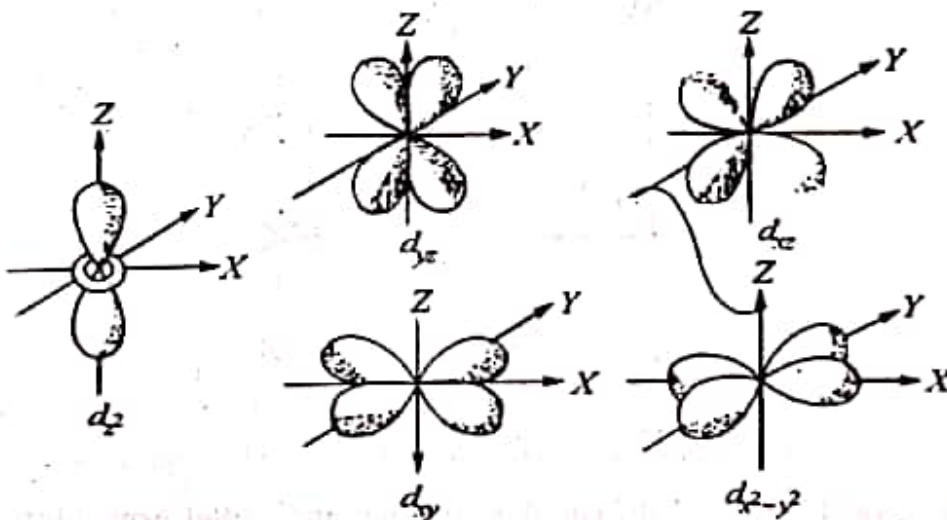


Fig. 1.19. Shapes of d -orbitals.